

FILE 'CASREACT' ENTERED AT 17:52:11 ON 12 JUN 2007  
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

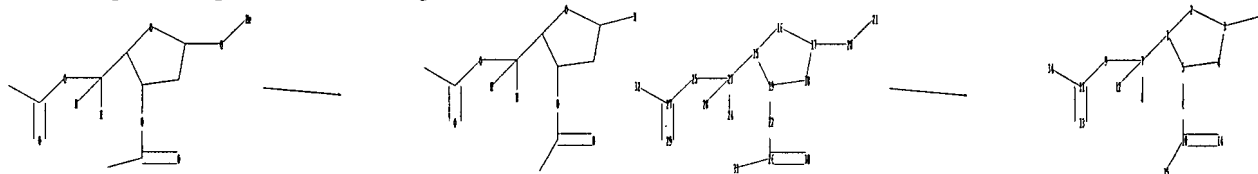
New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 12 million reactions
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>  
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction VI to I.str



chain nodes :  
6 7 8 9 10 11 12 13 14 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35  
ring nodes :  
1 2 3 4 5 15 16 17 18 19  
chain bonds :  
1-7 3-31 5-6 6-10 7-8 7-9 7-12 9-11 10-14 10-35 11-13 11-34 15-23 17-20 19-22 20-21  
22-26 23-24 23-25 23-28 25-27 26-30 26-33 27-29 27-32  
ring bonds :  
1-2 1-5 2-3 3-4 4-5 15-16 15-19 16-17 17-18 18-19  
exact/norm bonds :  
1-2 1-5 2-3 3-4 4-5 5-6 6-10 7-9 9-11 10-14 11-13 15-16 15-19 16-17 17-18 17-20 18-19  
19-22 22-26 23-25 25-27 26-30 27-29  
exact bonds :  
1-7 3-31 7-8 7-12 10-35 11-34 15-23 20-21 23-24 23-28 26-33 27-32

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS  
13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS  
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS  
34:CLASS 35:CLASS  
fragments assigned product role:  
containing 1  
fragments assigned reactant/reagent role:  
containing 15

L1 STRUCTURE UPLOADED

=> s l1  
SAMPLE SEARCH INITIATED 17:52:40 FILE 'CASREACT'  
SCREENING COMPLETE - 1 REACTIONS TO VERIFY FROM 1 DOCUMENTS  
100.0% DONE 1 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 1 TO 79  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 ( 0 REACTIONS)

=> s l1 full

FULL SEARCH INITIATED 17:52:43 FILE 'CASREACT'  
SCREENING COMPLETE - 144 REACTIONS TO VERIFY FROM 86 DOCUMENTS

100.0% DONE 144 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1 ( 0 REACTIONS)

=> file stng

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 113.55           | 113.76        |

FILE 'STNGUIDE' ENTERED AT 17:52:52 ON 12 JUN 2007  
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FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Jun 8, 2007 (20070608/UP).

=> file casreact

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 0.12             | 113.88        |

FILE 'CASREACT' ENTERED AT 17:53:48 ON 12 JUN 2007  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

New CAS Information Use Policies, enter HELP USAGETERMS for details.

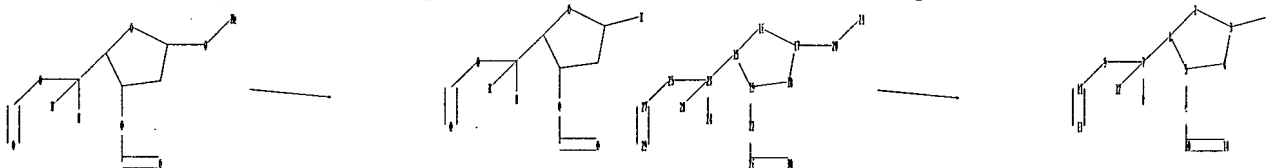
\*\*\*\*\*  
\* CASREACT now has more than 12 million reactions \*  
\* \*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

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=>

Uploading C:\Program Files\Stnexp\Queries\10578800\reaction VI to I acyl.str



chain nodes :  
6 7 8 9 10 11 12 13 14 20 21 22 23 24 25 26 27 28 29 30 31  
ring nodes :  
1 2 3 4 5 15 16 17 18 19  
chain bonds :  
1-7 3-31 5-6 6-10 7-8 7-9 7-12 9-11 10-14 11-13 15-23 17-20 19-22 20-21 22-26 23-24  
23-25 23-28 25-27 26-30 27-29

ring bonds :

1-2 1-5 2-3 3-4 4-5 15-16 15-19 16-17 17-18 18-19

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 5-6 6-10 7-9 9-11 10-14 11-13 15-16 15-19 16-17 17-18 17-20 18-19  
19-22 22-26 23-25 25-27 26-30 27-29

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Match level :

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13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS  
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> s l4

SAMPLE SEARCH INITIATED 17:54:10 FILE 'CASREACT'

SCREENING COMPLETE - 70 REACTIONS TO VERIFY FROM 18 DOCUMENTS

100.0% DONE 70 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED VERIFICATIONS: 899 TO 1901

PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4 ( 0 REACTIONS)

=> s l4 full

FULL SEARCH INITIATED 17:54:13 FILE 'CASREACT'

SCREENING COMPLETE - 4637 REACTIONS TO VERIFY FROM 461 DOCUMENTS

100.0% DONE 4637 VERIFIED 64 HIT RXNS 28 DOCS

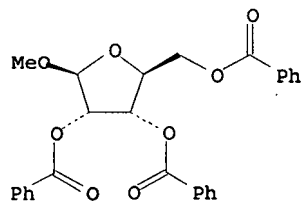
SEARCH TIME: 00.00.01

L6 28 SEA SSS FUL L4 ( .64 REACTIONS)

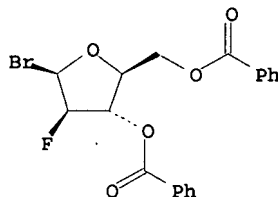
=> d l6 1-28

L6 ANSWER 1 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(86) OF 183 - 5 STEPS



1. Ac2O, H2SO4, Water, AcOH
2. HBr, Water, CH2Cl2
- 3.1. SO2Cl2, CH2Cl2, DMF
- 3.2. 1H-Imidazole
4. KHF2, HF, S:123513-85-9, Water
5. HBr, AcOH, CH2Cl2

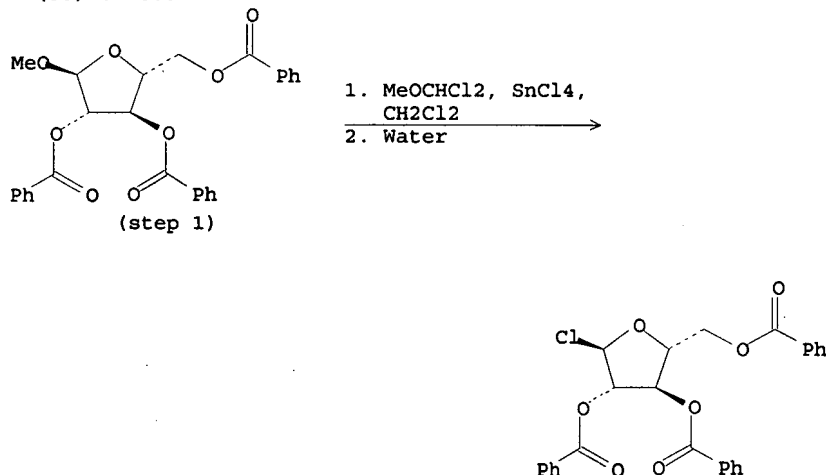


REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1891710, 10 Jan 2007

NOTE: 2) regioselective, 4) stereoselective, 5) regioselective, in the dark  
 CON: STEP(1.1) 0 deg C; 0 deg C -> room temperature; overnight, cooled  
 STEP(2.1) 3.5 hours, 0 deg C; 2 hours, room temperature  
 STEP(3.1) -15 deg C; 0.5 hours, -15 deg C;  
 -15 deg C -> room temperature; 4 hours, room temperature  
 STEP(3.2) 0 deg C; 17 hours, room temperature  
 STEP(4.1) room temperature -> 150 deg C; 150 deg C -> 160 deg C;  
 1 hour, 160 deg C  
 STEP(5) 24 hours, room temperature

L6 ANSWER 2 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

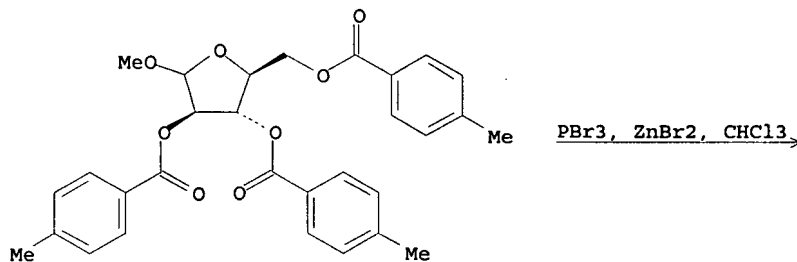
RX(35) OF 806



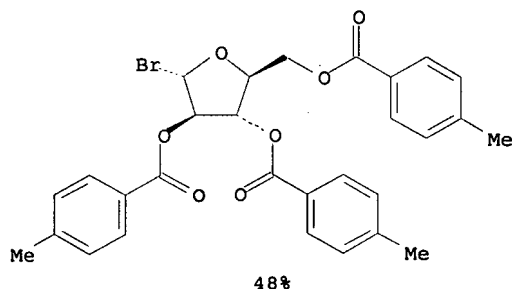
REF: Journal of Organic Chemistry, 71(21), 8071-8088; 2006  
 NOTE: regioselective  
 CON: STAGE(1) 13 hours, room temperature  
 STAGE(2) 45 minutes, room temperature

L6 ANSWER 3 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 17

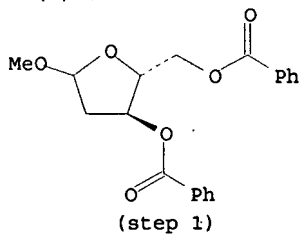


RX(1) OF 17

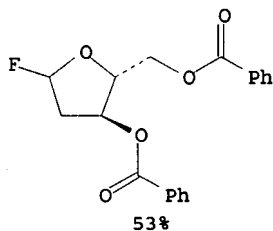


REF: Eur. Pat. Appl., 1705181, 27 Sep 2006  
 CON: 19 hours, 45 deg C

RX(2) OF 21



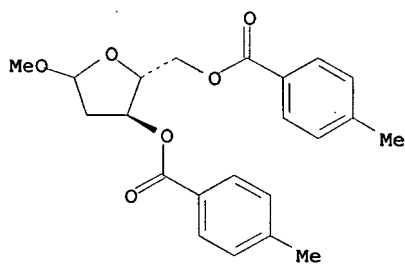
1. HCl, Water,  
Dioxane
2. DAST [(Et<sub>2</sub>N).SF<sub>3</sub>],  
THF
3. MeOH



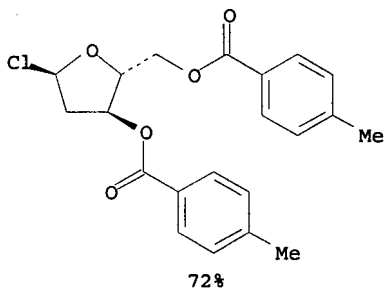
REF: Journal of the American Chemical Society, 127(44), 15612-15617; 2005

CON: STAGE(1) 1 hour, reflux  
STAGE(2) -78 deg C; 20 minutes, room temperature  
STAGE(3) room temperature

RX(2) OF 33



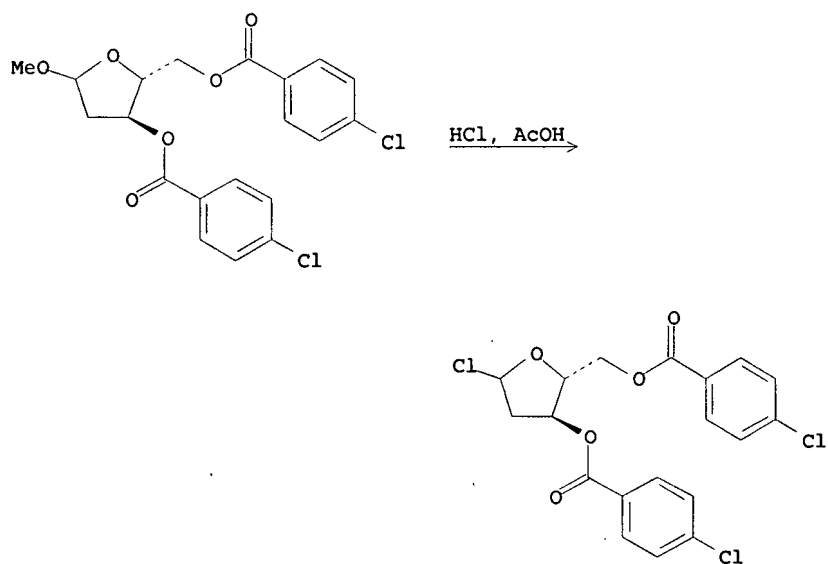
HCl, Et<sub>2</sub>O



REF: Organic Letters, 7(14), 2853-2856; 2005

NOTE: stereoselective  
CON: 10 minutes, 0 deg C

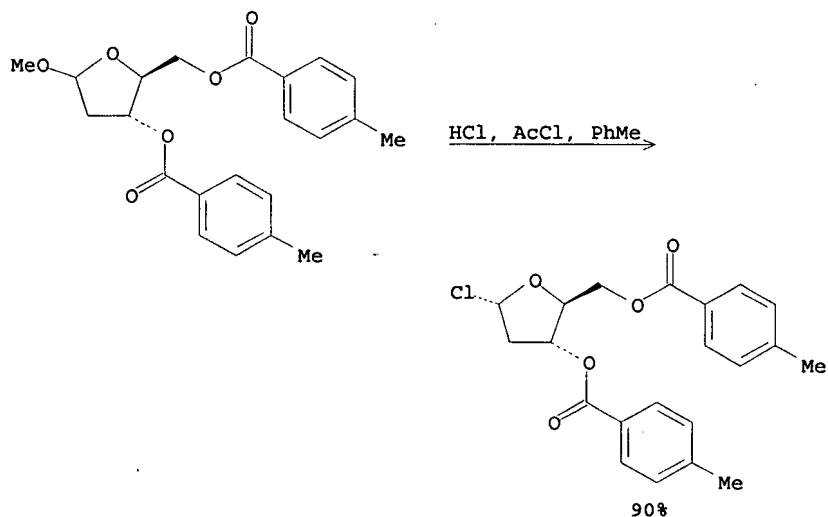
RX(4) OF 21



REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1539845, 27 Oct 2004  
CON: 2 - 4 hours, 30 deg C

L6 ANSWER 7 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(6) OF 24

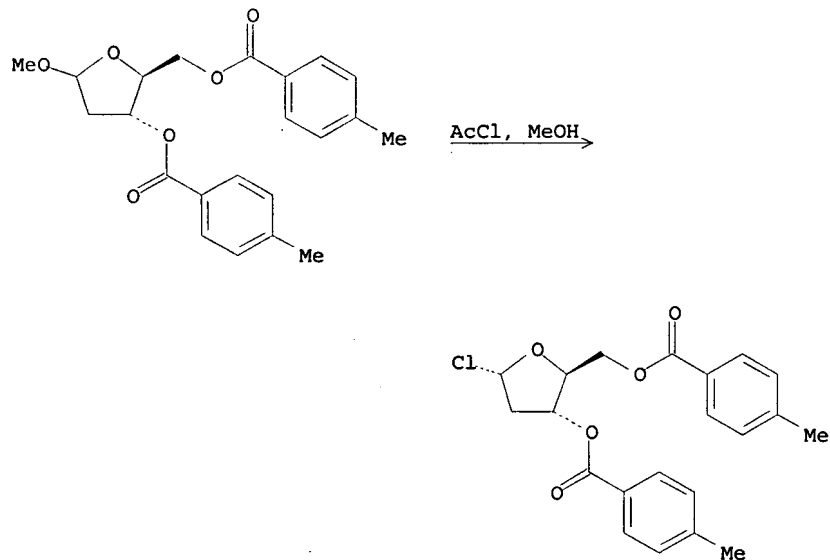


REF: PCT Int. Appl., 2005044832, 19 May 2005

CON: STAGE(1) room temperature; room temperature  $\rightarrow$  5 deg C;  
<15 deg C; 1 hour, 5 deg C

L6 ANSWER 8 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 32



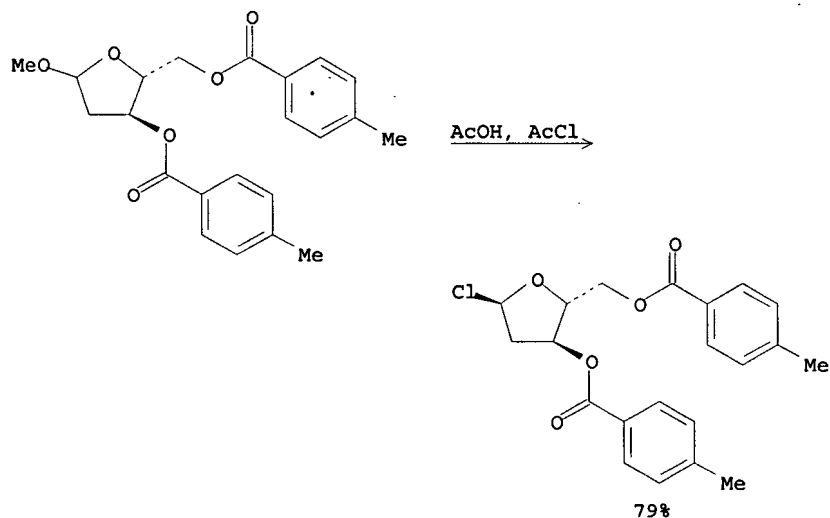
REF: U.S. Pat. Appl. Publ., 2004266996, 30 Dec 2004

NOTE: workup

CON: STAGE(1) room temperature; room temperature -> 10 deg C;  
3.5 - 4 hours, 8 - 10 deg C; 4 hours, 8 - 10 deg C

L6 ANSWER 9 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 64



79%

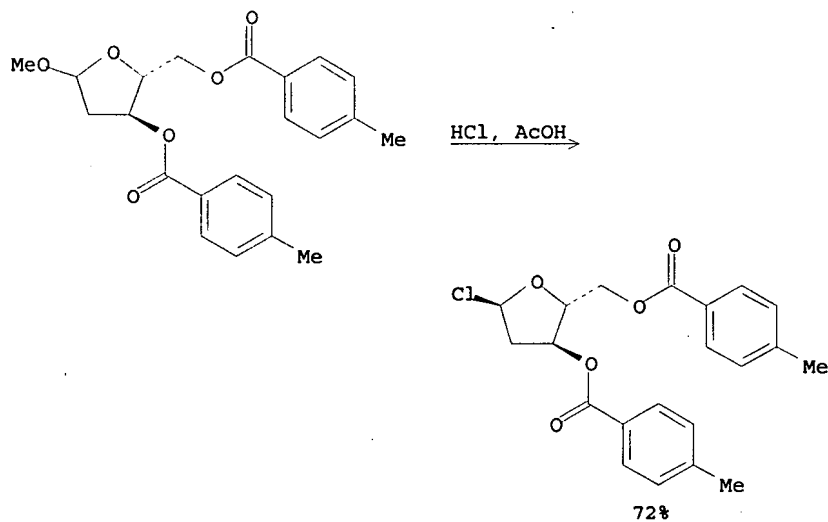
REF: Organic & Biomolecular Chemistry, 1(13), 2267-2275; 2003

NOTE: stereoselective

CON: room temperature

L6 ANSWER 10 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(4) OF 34

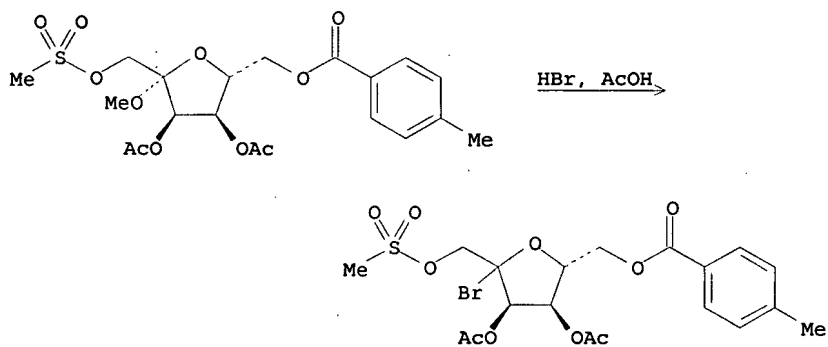


REF: Organic Letters, 4(26), 4571-4574; 2002

CON: STAGE(1) 5 minutes, room temperature; 1 hour, 10 deg C

L6 ANSWER 11 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(10) OF 74



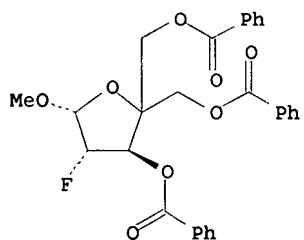
REF: Tetrahedron Letters, 43(37), 6553-6555; 2002

CON: 1 - 3 hour, 20 deg C

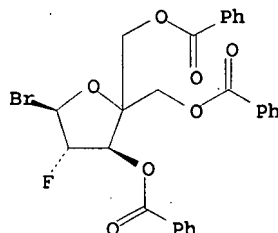
L6 ANSWER 12 OF 28 CASREACT COPYRIGHT 2007 ACS on STN



RX(57) OF 206 - 3 STEPS



1. F3CCO2H, Water  
2. Ac2O, Pyridine  
3. HBr, AcOH

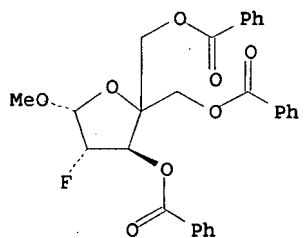


REF: Nucleosides, Nucleotides & Nucleic Acids, 20(4-7), 747-750; 2001

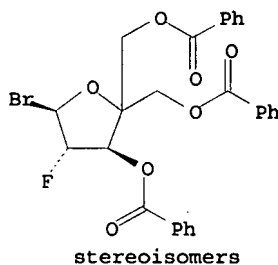
NOTE: 1) stereoselective, 2:1 alpha:beta, 2) stereoselective, 3:1 alpha:beta, 3) stereoselective, 6:1 alpha:beta

L6 ANSWER 13 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(62) OF 180 - 3 STEPS



1.1. F3CCO2H, Water  
1.2. NaHCO3, Water  
2. Ac2O, Pyridine  
3. HBr, CH2Cl2, AcOH

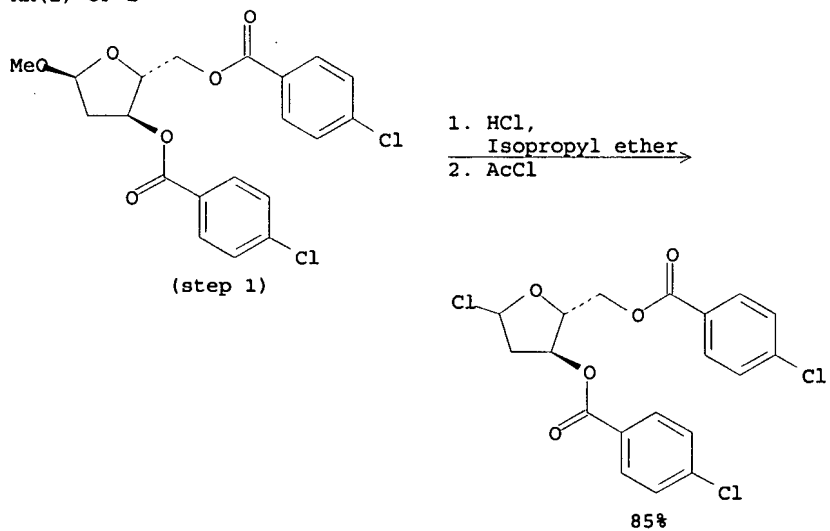


REF: Nucleosides, Nucleotides & Nucleic Acids, 20(8), 1583-1598; 2001

NOTE: 1) 67:33 alpha:beta, stereoselective, 2) stereoselective, 3) 86:14 alpha:beta, stereoselective

L6 ANSWER 14 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

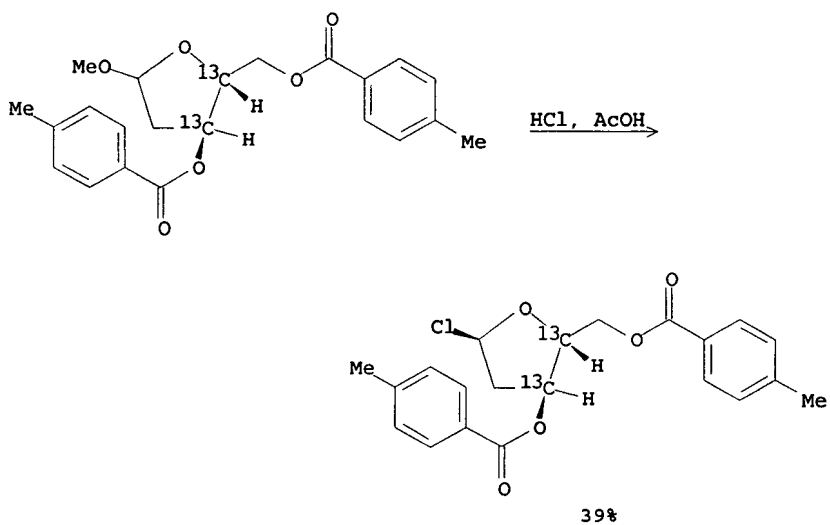
RX(1) OF 1



REF: Jpn. Kokai Tokkyo Koho, 2000290289, 17 Oct 2000

L6 ANSWER 15 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(10) OF 66



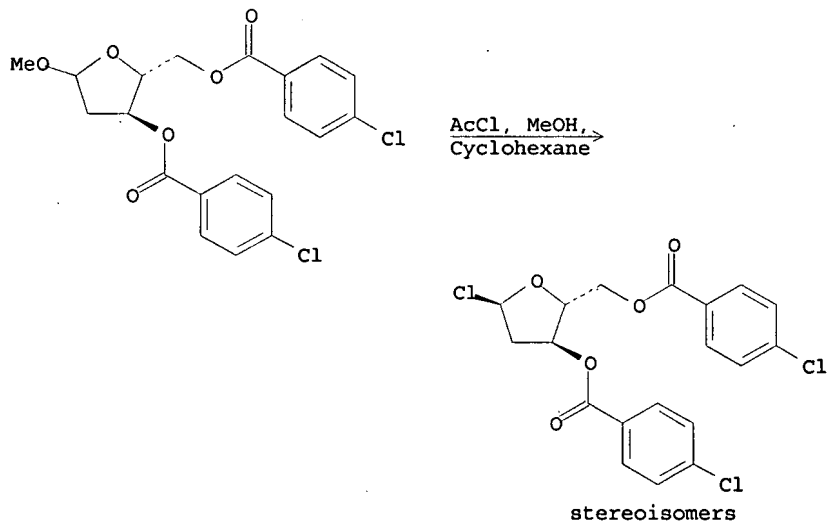
REF: European Journal of Organic Chemistry, (5), 861-866; 2000

NOTE: gaseous HCl used

CON: STAGE(1) 0 deg C; 10 minutes

L6 ANSWER 16 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 8

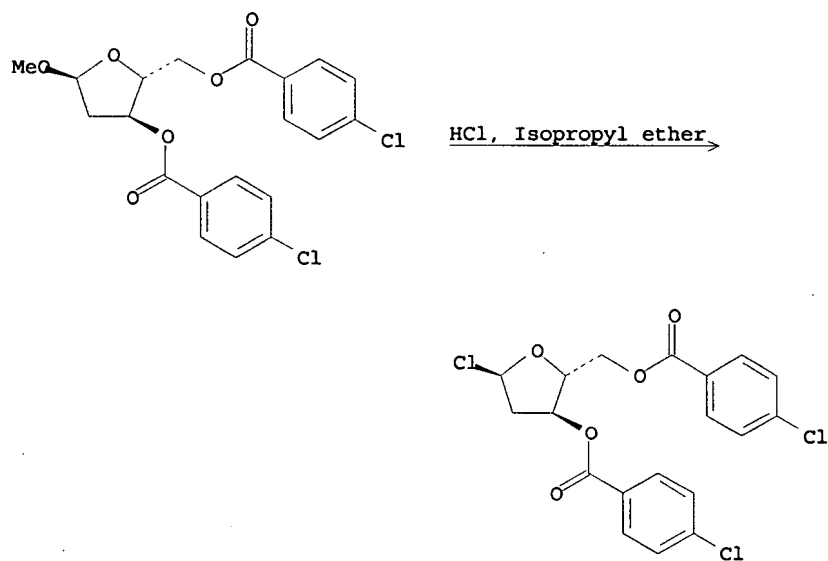


REF: Jpn. Kokai Tokkyo Koho, 07224081, 22 Aug 1995, Heisei

NOTE: 25.degree. for 4 h; 84.8% yield

L6 ANSWER 17 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

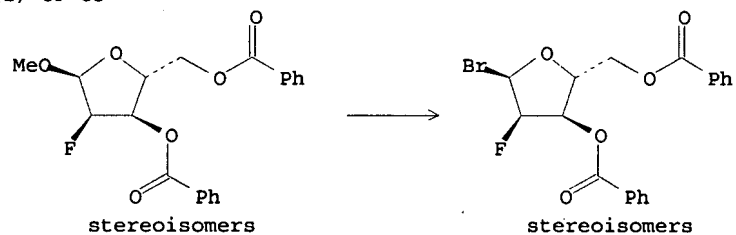
RX(7) OF 28



REF: Eur. Pat. Appl., 635517, 25 Jan 1995

L6 ANSWER 18 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

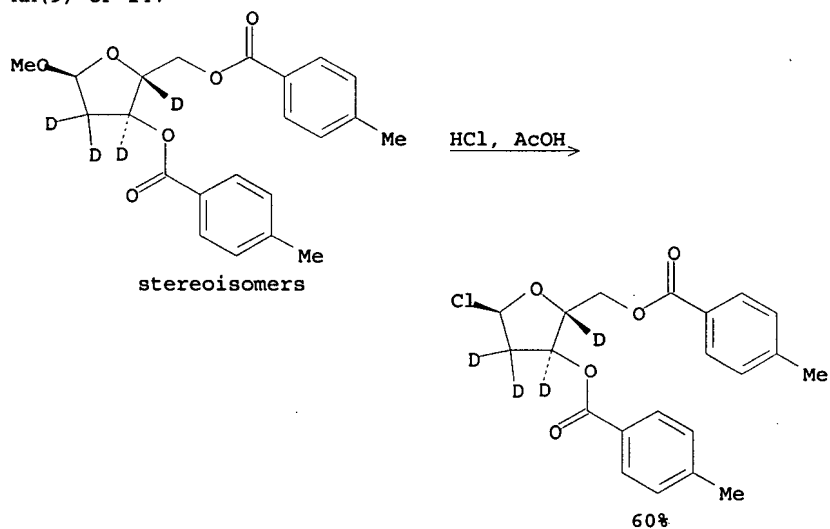
RX(1) OF 83



REF: PCT Int. Appl., 9310137, 27 May 1993  
NOTE: 2 STEPS

L6 ANSWER 19 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

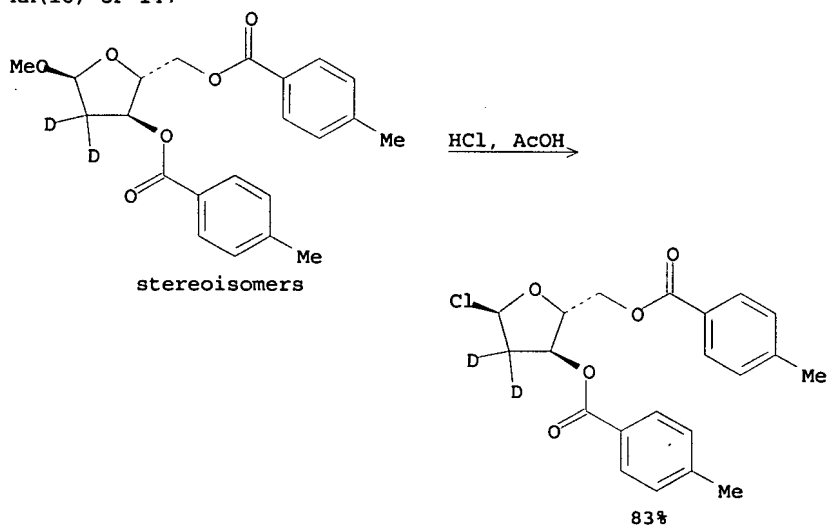
RX(9) OF 147



REF: Tetrahedron, 43(18), 4227-34; 1987

L6 ANSWER 20 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

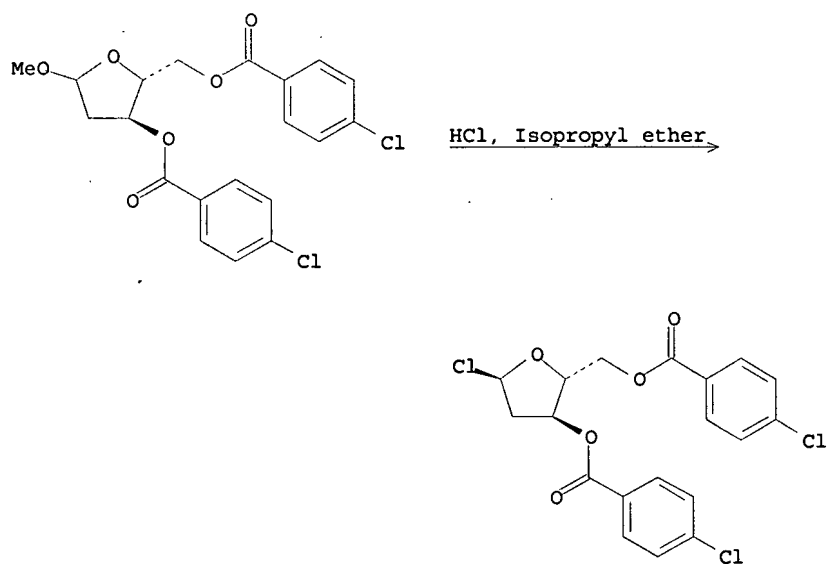
RX(18) OF 147



REF: Tetrahedron, 43(10), 2355-68; 1987

L6 ANSWER 21 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

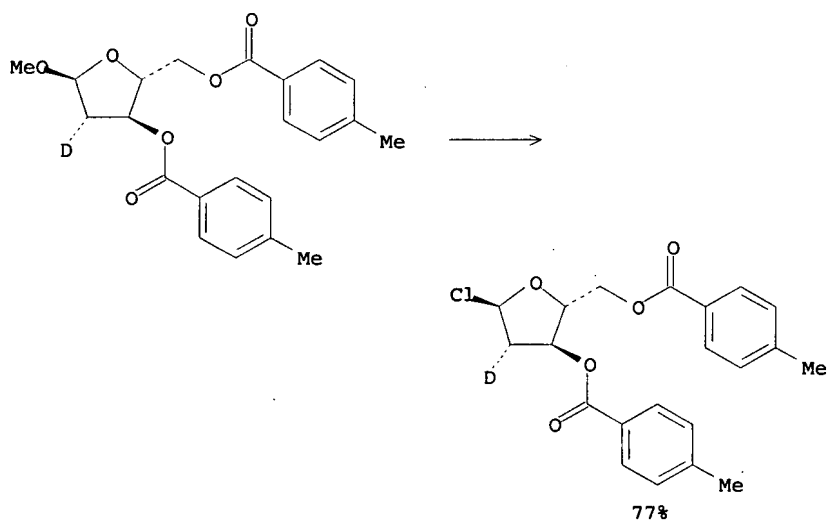
RX(2) OF 88



REF: Nippon Kagaku Kaishi, (12), 1765-70; 1986

L6 ANSWER 22 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

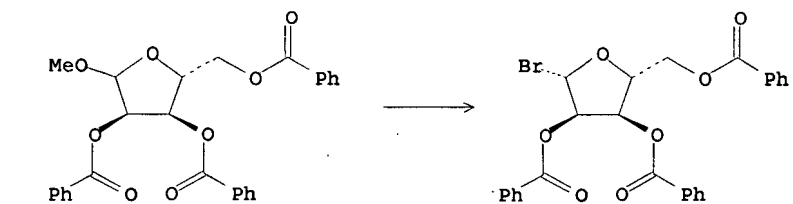
RX(6) OF 177



REF: Tetrahedron, 42(19), 5427-41; 1986

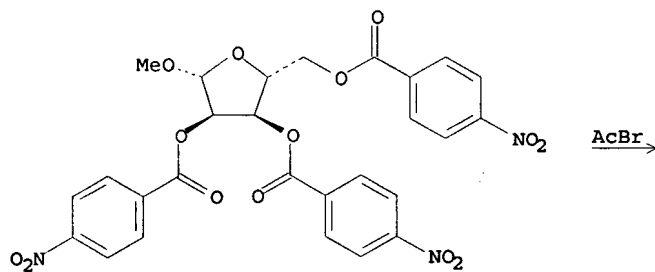
L6 ANSWER 23 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 5

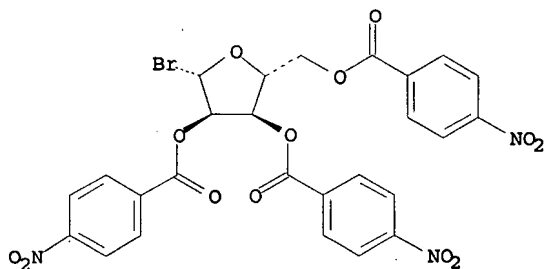


REF: Eur. Pat. Appl., 145978, 26 Jun 1985

RX(2) OF 3

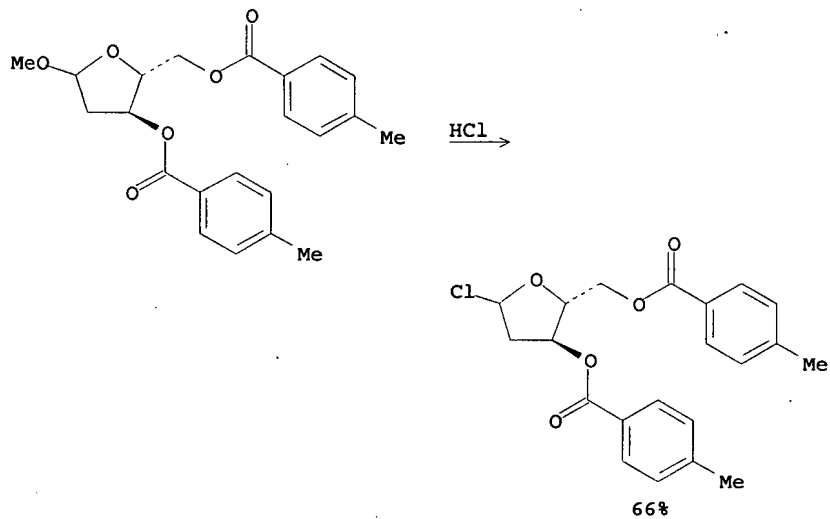


RX(2) OF 3



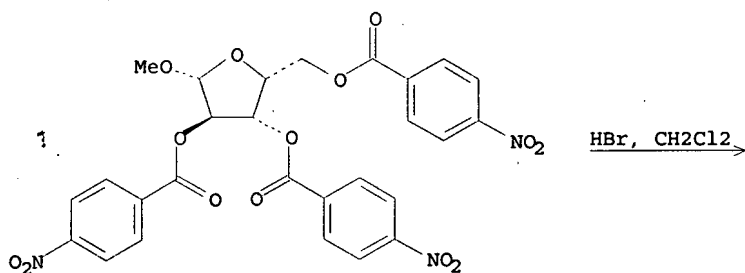
REF: U.S., 4282349, 04 Aug 1981

RX(1) OF 51

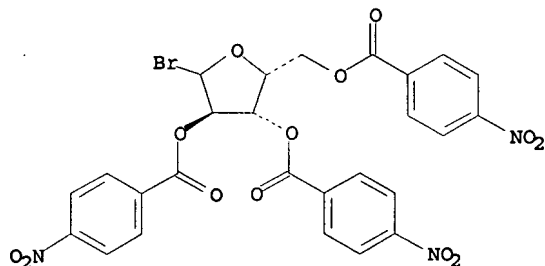


REF: U.S., 4239753, 16 Dec 1980

RX(1) OF 1



RX(1) OF 1



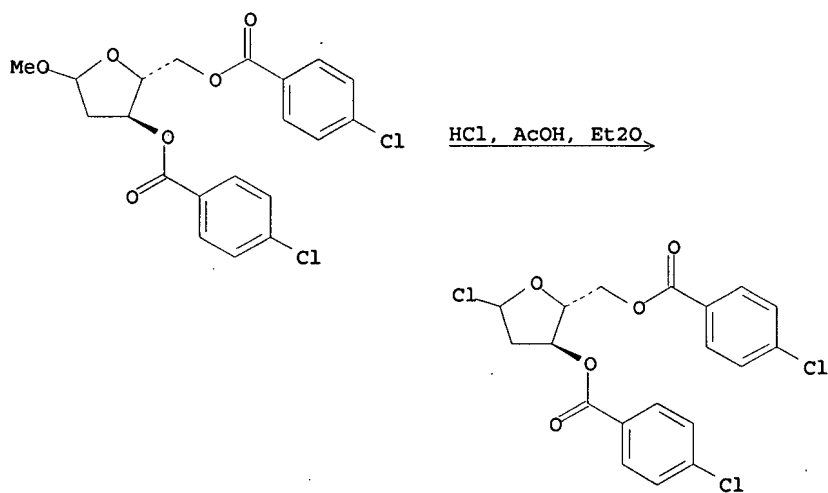
68%

REF: Carbohydrate Research, 47(2), 233-40; 1976

NOTE: Classification: Substitution; Bromination; # Conditions: HBr  
CH<sub>2</sub>Cl<sub>2</sub>; 24h 0-3 deg

L6 ANSWER 27 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 13



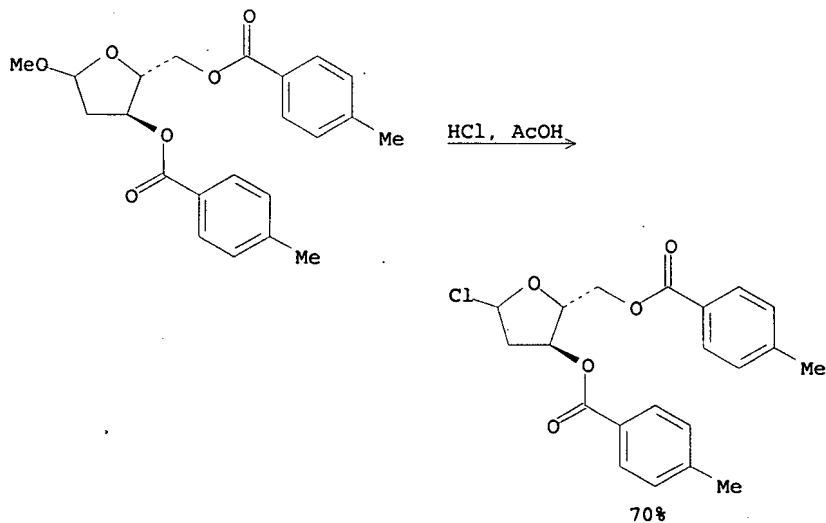
65%

REF: Journal of the American Chemical Society, 83,, 4066-50; 1961

NOTE: Classification: Substitution; Chlorination; # Conditions: HCl  
Et<sub>2</sub>O AcOH

L6 ANSWER 28 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 3



REF: Journal of the American Chemical Society, 81,, 4112-13; 1959

NOTE: Classification: Substitution; Chlorination; # Conditions: HCl  
AcOH

=> d his

(FILE 'HOME' ENTERED AT 17:52:00 ON 12 JUN 2007)

FILE 'CASREACT' ENTERED AT 17:52:11 ON 12 JUN 2007

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

FILE 'STNGUIDE' ENTERED AT 17:52:52 ON 12 JUN 2007

FILE 'CASREACT' ENTERED AT 17:53:48 ON 12 JUN 2007

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 28 S L4 FULL

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

194.08

307.96

STN INTERNATIONAL LOGOFF AT 17:54:44 ON 12 JUN 2007



FILE 'CASREACT' ENTERED AT 17:59:12 ON 12 JUN 2007  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

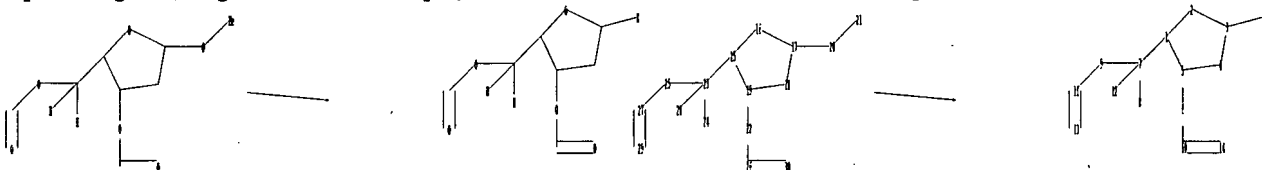
New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 12 million reactions
*
*****
```

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=>  
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction VI to I acyl.str



```
chain nodes :
6 7 8 9 10 11 12 13 14 20 21 22 23 24 25 26 27 28 29 30 31
ring nodes :
1 2 3 4 5 15 16 17 18 19
chain bonds :
1-7 3-31 5-6 6-10 7-8 7-9 7-12 9-11 10-14 11-13 15-23 17-20 19-22 20-21 22-26 23-24
23-25 23-28 25-27 26-30 27-29
ring bonds :
1-2 1-5 2-3 3-4 4-5 15-16 15-19 16-17 17-18 18-19
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-10 7-9 9-11 10-14 11-13 15-16 15-19 16-17 17-18 17-20 18-19
19-22 22-26 23-25 25-27 26-30 27-29
exact bonds :
1-7 3-31 7-8 7-12 15-23 20-21 23-24 23-28
```

```
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS
```

L1 STRUCTURE UPLOADED

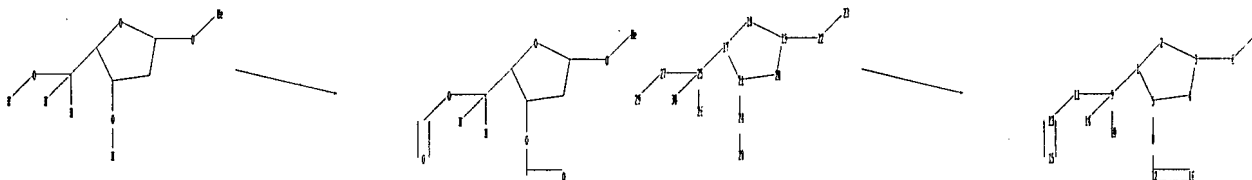
=> s l1 full

FULL SEARCH INITIATED 17:59:29 FILE 'CASREACT'  
SCREENING COMPLETE - 4637 REACTIONS TO VERIFY FROM 461 DOCUMENTS

100.0% DONE 4637 VERIFIED 64 HIT RXNS 28 DOCS  
SEARCH TIME: 00.00.01

L2 28 SEA SSS FUL L1 ( 64 REACTIONS)

=>  
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction V to VI.str



chain nodes :  
 6 7 8 9 10 11 12 13 14 15 16 22 23 24 25 26 27 28 29 30  
 ring nodes :  
 1 2 3 4 5 17 18 19 20 21  
 chain bonds :  
 1-9 3-6 5-8 6-7 8-12 9-10 9-11 9-14 11-13 12-16 13-15 17-25 19-22 21-24 22-23 24-28  
 25-26 25-27 25-30 27-29  
 ring bonds :  
 1-2 1-5 2-3 3-4 4-5 17-18 17-21 18-19 19-20 20-21  
 exact/norm bonds :  
 1-2 1-5 2-3 3-4 3-6 4-5 5-8 8-12 9-11 11-13 12-16 13-15 17-18 17-21 18-19 19-20 19-22  
 20-21 21-24 25-27  
 exact bonds :  
 1-9 6-7 9-10 9-14 17-25 22-23 24-28 25-26 25-30 27-29

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS  
 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS 23:CLASS  
 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS  
 fragments assigned product role:  
 containing 1  
 fragments assigned reactant/reagent role:  
 containing 17

L3 STRUCTURE UPLOADED

=> s l3  
 SAMPLE SEARCH INITIATED 17:59:52 FILE 'CASREACT'  
 SCREENING COMPLETE - 581 REACTIONS TO VERIFY FROM 45 DOCUMENTS  
 100.0% DONE 581 VERIFIED 2 HIT RXNS 2 DOCS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED VERIFICATIONS: 10175 TO 13065  
 PROJECTED ANSWERS: 2 TO 124

L4 2 SEA SSS SAM L3 ( 2 REACTIONS)

=> s l3 full  
 FULL SEARCH INITIATED 17:59:55 FILE 'CASREACT'  
 SCREENING COMPLETE - 11450 REACTIONS TO VERIFY FROM 894 DOCUMENTS  
 100.0% DONE 11450 VERIFIED 66 HIT RXNS 43 DOCS  
 SEARCH TIME: 00.00.01

L5 43 SEA SSS FUL L3 ( 66 REACTIONS)

=> d his

(FILE 'HOME' ENTERED AT 17:59:06 ON 12 JUN 2007)

FILE 'CASREACT' ENTERED AT 17:59:12 ON 12 JUN 2007

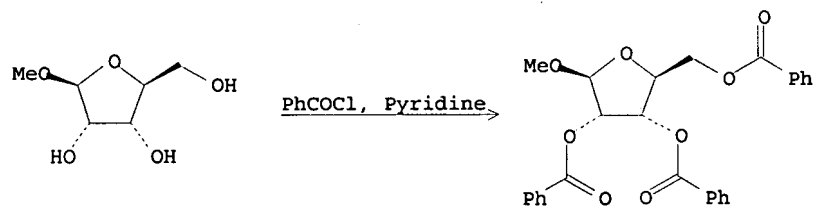
L1 STRUCTURE UPLOADED  
 L2 28 S L1 FULL  
 L3 STRUCTURE UPLOADED  
 L4 2 S L3  
 L5 43 S L3 FULL

=> s l2 and l5  
 L6 13 L2 AND L5

=> d 16 1-13

L6 ANSWER 1 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 183

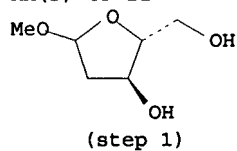


REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1891710, 10 Jan 2007

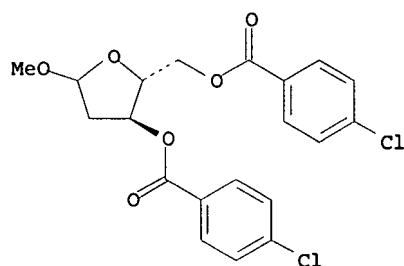
CON: STAGE(1) 0 deg C; 17 hours, room temperature

L6 ANSWER 2 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 21



1. 4-ClC<sub>6</sub>H<sub>4</sub>COCl  
2. Water, CH<sub>2</sub>Cl<sub>2</sub>

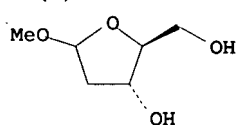


REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1539845, 27 Oct 2004

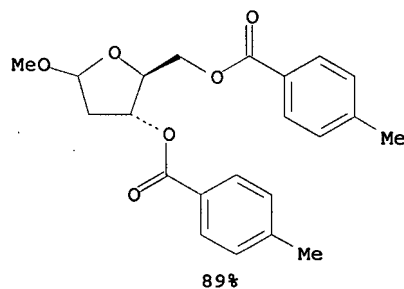
CON: STAGE(1) 4 - 5 hours, 40 deg C  
STAGE(2) 0.5 hours, 5 - 10 deg C

L6 ANSWER 3 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

RX(4) OF 24



4-MeC<sub>6</sub>H<sub>4</sub>COCl, Et<sub>3</sub>N,  
PhMe

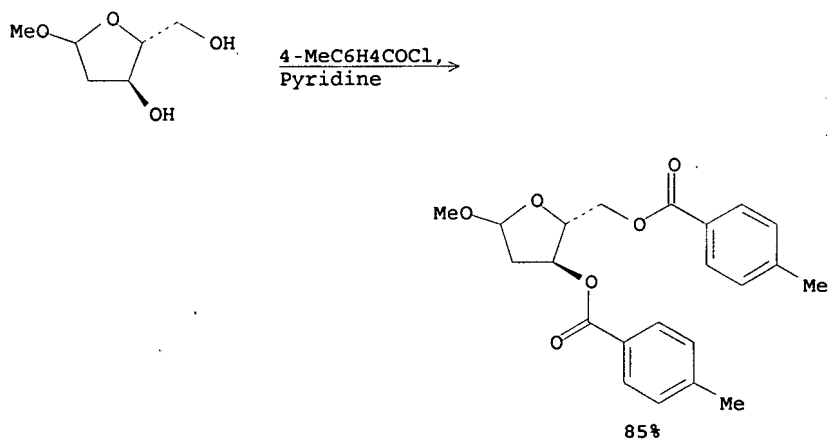


REF: PCT Int. Appl., 2005044832, 19 May 2005

CON: STAGE(1) room temperature -> 40 deg C; 40 deg C -> 60 deg C;  
5 hours, 60 deg C

L6 ANSWER 4 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

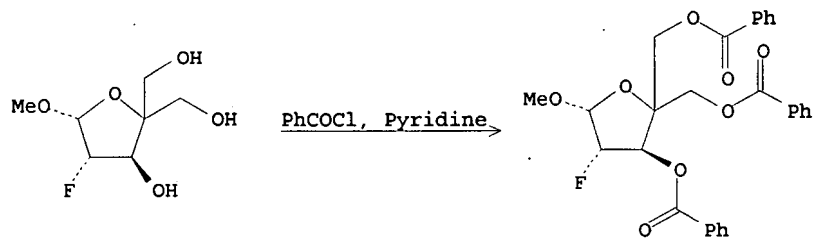
RX(2) OF 34



REF: Organic Letters, 4(26), 4571-4574; 2002  
CON: STAGE(1) 0 deg C; overnight, room temperature

L6 ANSWER 5 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

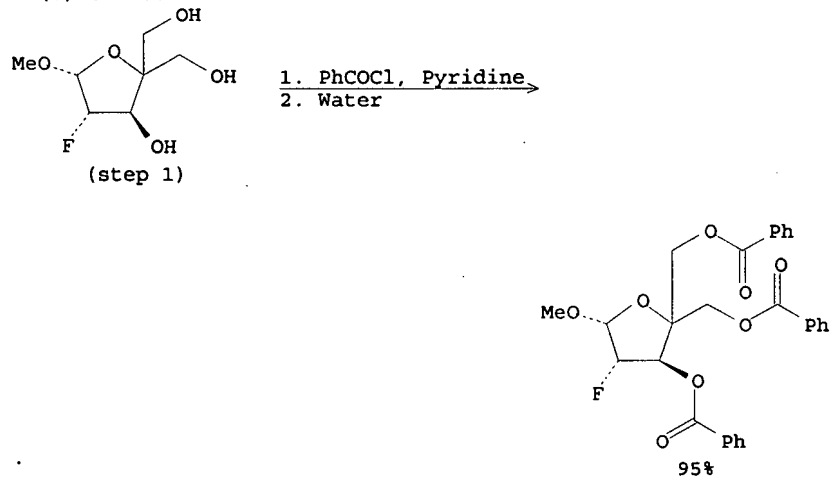
RX(8) OF 206



REF: Nucleosides, Nucleotides & Nucleic Acids, 20(4-7), 747-750;  
2001  
NOTE: stereoselective

L6 ANSWER 6 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

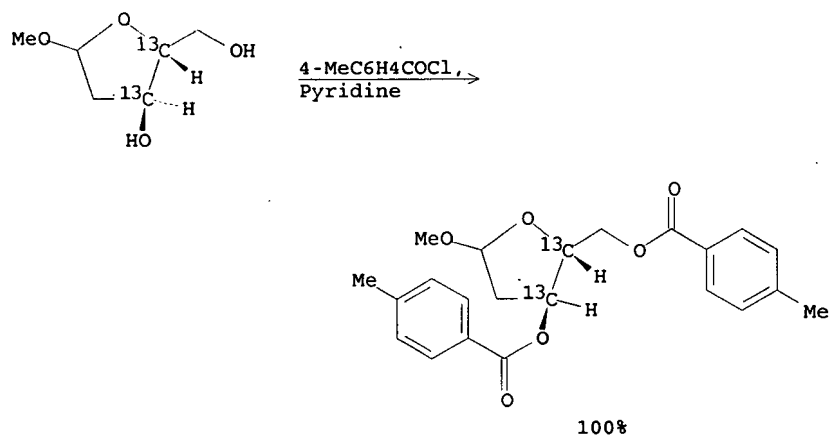
RX(8) OF 180



REF: Nucleosides, Nucleotides & Nucleic Acids, 20(8), 1583-1598;  
2001

L6 ANSWER 7 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

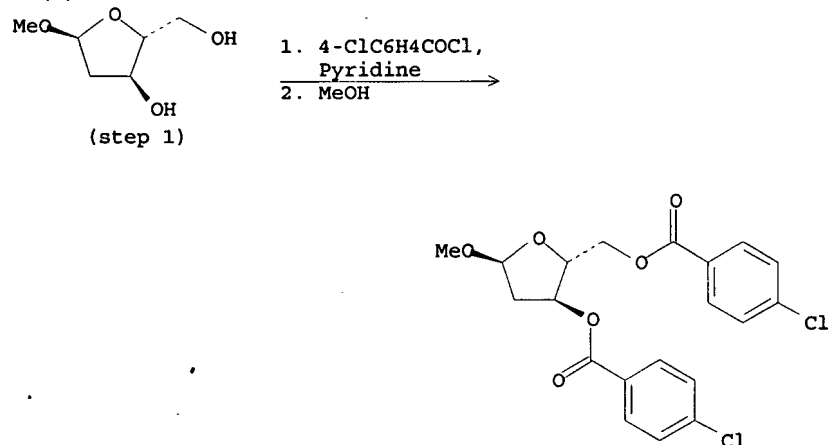
RX(9) OF 66



REF: European Journal of Organic Chemistry, (5), 861-866; 2000  
CON: 2 hours, 40 deg C

L6 ANSWER 8 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

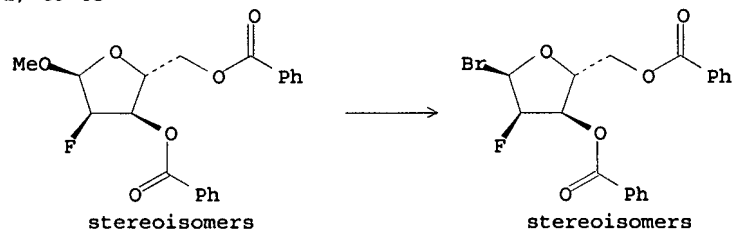
RX(6) OF 28



REF: Eur. Pat. Appl., 635517, 25 Jan 1995

L6 ANSWER 9 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

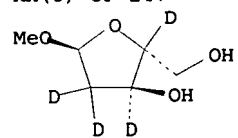
RX(1) OF 83



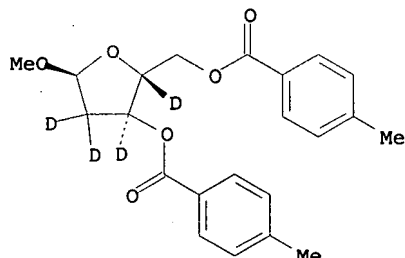
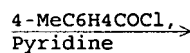
REF: PCT Int. Appl., 9310137, 27 May 1993  
NOTE: 2 STEPS

L6 ANSWER 10 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

RX(8) OF 147



stereoisomers

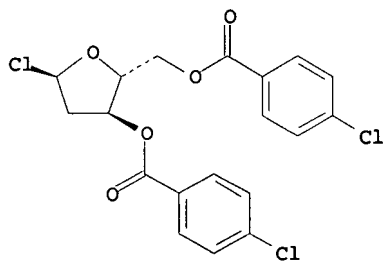
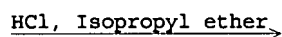
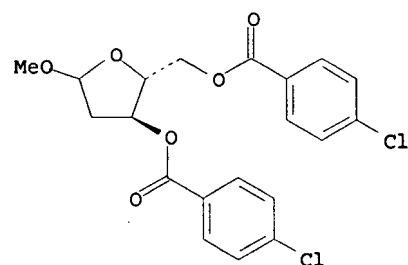


stereoisomers

REF: Tetrahedron, 43(18), 4227-34; 1987  
NOTE: 87% overall

L6 ANSWER 11 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

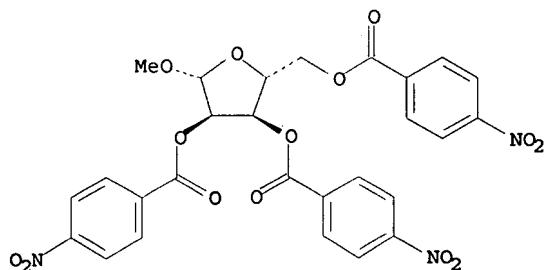
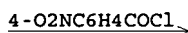
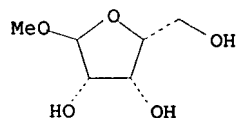
RX(2) OF 88



REF: Nippon Kagaku Kaishi, (12), 1765-70; 1986

L6 ANSWER 12 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

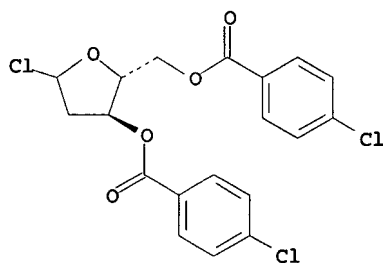
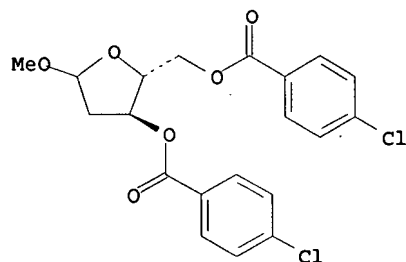
RX(1) OF 3



REF: U.S., 4282349, 04 Aug 1981

L6 ANSWER 13 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 13



65%

REF: Journal of the American Chemical Society, 83,, 4066-50; 1961

NOTE: Classification: Substitution; Chlorination; # Conditions: HCl  
Et2O AcOH

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE

ENTRY

264.73

TOTAL

SESSION

264.94

STN INTERNATIONAL LOGOFF AT 18:00:49 ON 12 JUN 2007

FILE 'CASREACT' ENTERED AT 15:44:56 ON 12 JUN 2007  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

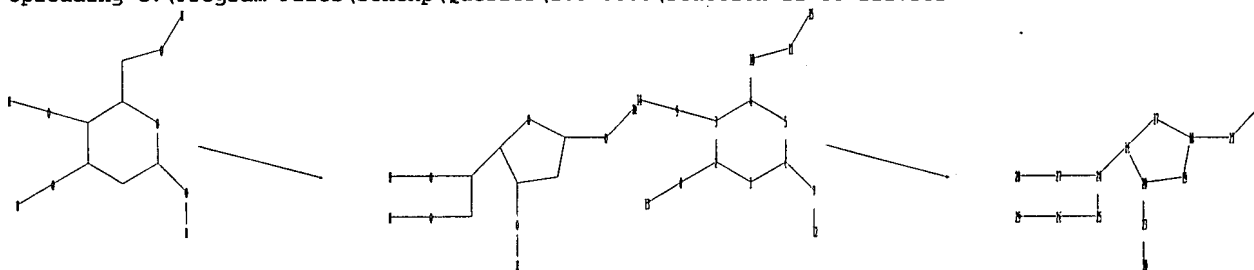
New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 12 million reactions
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>  
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction II to III.str



```
chain nodes :
7 8 9 10 11 12 13 14 15 21 22 23 24 25 26 27 28 29 30
ring nodes :
1 2 3 4 5 6 16 17 18 19 20
chain bonds :
2-8 3-9 4-10 6-7 7-12 8-13 9-14 10-11 11-15 16-24 18-21 20-23 21-22 23-30 24-25 24-27
25-26 26-29 27-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-6 2-3 2-8 3-4 3-9 4-5 5-6 6-7 10-11 16-17 16-20 17-18 18-19 18-21 19-20 20-23
24-27 25-26
exact bonds :
4-10 7-12 8-13 9-14 11-15 16-24 21-22 23-30 24-25 26-29 27-28
```

```
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
fragments assigned product role:
containing 16
fragments assigned reactant/reagent role:
containing 1
```

L1 STRUCTURE UPLOADED

=> d



L1 HAS NO ANSWERS  
L1 STR  
\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> s l1  
SAMPLE SEARCH INITIATED 15:45:15 FILE 'CASREACT'  
SCREENING COMPLETE - 522 REACTIONS TO VERIFY FROM 17 DOCUMENTS  
100.0% DONE 522 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 9070 TO 11810  
PROJECTED ANSWERS: 0 TO 0

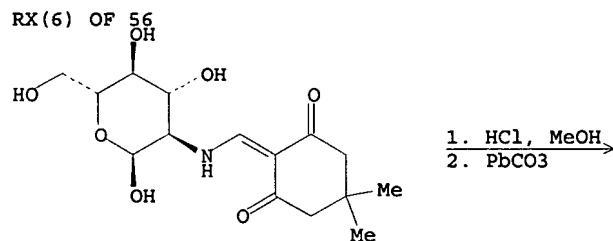
L2 0 SEA SSS SAM L1 ( 0 REACTIONS)

=> s l1 full  
FULL SEARCH INITIATED 15:45:23 FILE 'CASREACT'  
SCREENING COMPLETE - 7531 REACTIONS TO VERIFY FROM 254 DOCUMENTS  
100.0% DONE 7531 VERIFIED 6 HIT RXNS 3 DOCS  
SEARCH TIME: 00.00.02

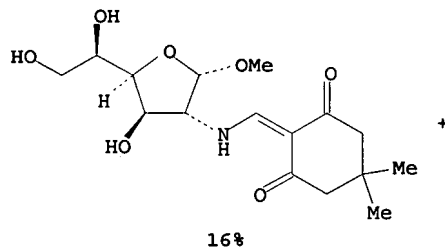
L3 3 SEA SSS FUL L1 ( 6 REACTIONS)

=> d l3 1-3

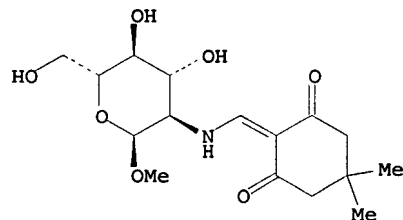
L3 ANSWER 1 OF 3 CASREACT COPYRIGHT 2007 ACS on STN



(step 1)  
stereoisomers



RX(6) OF 56

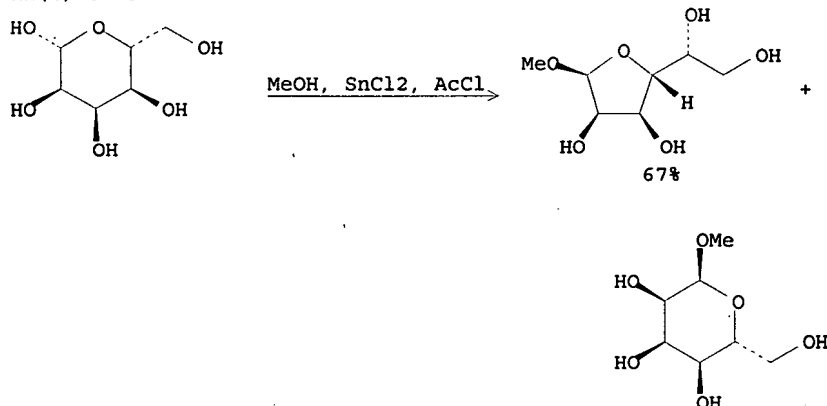


stereoisomers

REF: Carbohydrate Research, 162(2), 181-97; 1987

L3 ANSWER 2 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 3

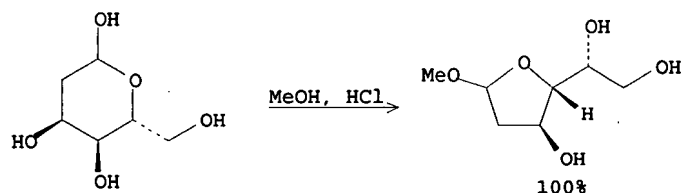


REF: Carbohydrate Research, 25(1), 43-8; 1972

NOTE: Classification: Heterocycle formation; Ring cleavage; Hydrolysis; Alkoxylation; # Conditions: SnCl<sub>2</sub> AcCl; Rf 200nm; # Comments: yield for alpha anomer of 5-membered ring. 14% yield for; beta anomer. 6% yield for alpha anomer of 6-membered ring; product. 8% yield for beta anomer

L3 ANSWER 3 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1



REF: Chemical Communications (London), (14), 808-9; 1968

NOTE: Classification: Alkoxylation; Acetalisation; Ring contraction; # Conditions: MeOH HCl 6mn 20 deg; # Comments: alpha/beta=1/1 for product

=> d his

(FILE 'HOME' ENTERED AT 15:44:45 ON 12 JUN 2007)

FILE 'CASREACT' ENTERED AT 15:44:56 ON 12 JUN 2007

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 3 S L1 FULL

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

122.13

122.34

STN INTERNATIONAL LOGOFF AT 15:45:46 ON 12 JUN 2007

FILE 'CASREACT' ENTERED AT 16:48:14 ON 12 JUN 2007  
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

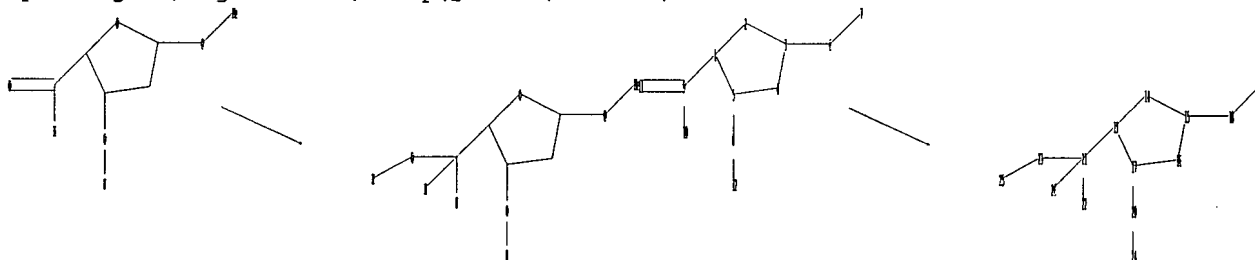
New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 12 million reactions
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>  
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction iv to v.str



```
chain nodes :
6 7 8 9 10 11 12 18 19 20 21 22 23 24 25 26
ring nodes :
1 2 3 4 5 13 14 15 16 17
chain bonds :
1-9 3-6 5-8 6-7 8-12 9-10 9-11 13-21 15-18 17-20 18-19 20-24 21-22 21-23 21-26 23-25
ring bonds :
1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 2-3 3-4 3-6 4-5 5-8 9-11 13-14 13-17 14-15 15-16 15-18 16-17 17-20 21-23
exact bonds :
1-9 6-7 8-12 9-10 13-21 18-19 20-24 21-22 21-26 23-25
```

```
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS
fragments assigned product role:
containing 13
fragments assigned reactant/reagent role:
containing 1
```

L1 STRUCTURE UPLOADED

```
=> d
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
```

Structure attributes must be viewed using STN Express query preparation.

=> s ;1  
ENTER LOGIC EXPRESSION, QUERY NAME, OR (END):end  
SEARCH ENDED BY USER

L2 407826 1

=> s 11  
SAMPLE SEARCH INITIATED 16:48:44 FILE 'CASREACT'  
SCREENING COMPLETE - 1397 REACTIONS TO VERIFY FROM 100 DOCUMENTS  
  
100.0% DONE 1397 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 25700 TO 30180  
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L1 ( 0 REACTIONS)

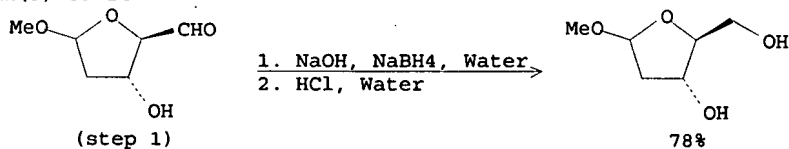
=> s 11 full  
FULL SEARCH INITIATED 16:48:49 FILE 'CASREACT'  
SCREENING COMPLETE - 32058 REACTIONS TO VERIFY FROM 1917 DOCUMENTS  
  
100.0% DONE 32058 VERIFIED 1 HIT RXNS 1 DOCS  
SEARCH TIME: 00.00.03

L4 1 SEA SSS FUL L1 ( 1 REACTIONS)

=> d 14

L4 ANSWER 1 OF 1 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 24



REF: PCT Int. Appl., 2005044832, 19 May 2005  
CON: STAGE(1) room temperature -> 0 deg C; <15 deg C; 30 minutes,  
cooled  
STAGE(2) pH 7

=>  
---Logging off of STN---

=>  
Executing the logoff script...

=> LOG Y

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 118.78           | 118.99        |

STN INTERNATIONAL LOGOFF AT 16:49:38 ON 12 JUN 2007

FILE 'CASREACT' ENTERED AT 16:44:50 ON 12 JUN 2007  
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

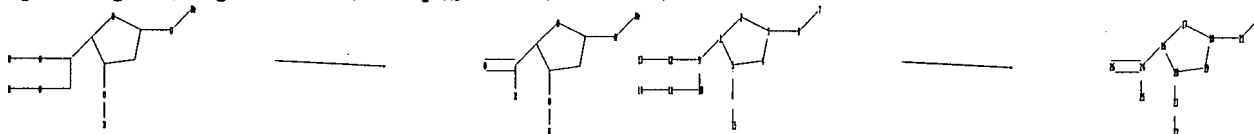
New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 12 million reactions
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>  
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction III to IV.str



chain nodes :  
6 7 8 9 10 11 12 13 14 15 21 22 23 24 25 26 27  
ring nodes :  
1 2 3 4 5 16 17 18 19 20  
chain bonds :  
1-9 3-6 5-8 6-7 8-15 9-10 9-12 10-11 11-14 12-13 16-24 18-21 20-23 21-22 23-27 24-25  
24-26  
ring bonds :  
1-2 1-5 2-3 3-4 4-5 16-17 16-20 17-18 18-19 19-20  
exact/norm bonds :  
1-2 1-5 2-3 3-4 3-6 4-5 5-8 9-12 10-11 16-17 16-20 17-18 18-19 18-21 19-20 20-23 24-26  
exact bonds :  
1-9 6-7 8-15 9-10 11-14 12-13 16-24 21-22 23-27 24-25

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS  
13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 22:CLASS 23:CLASS  
24:CLASS 25:CLASS 26:CLASS 27:CLASS  
fragments assigned product role:  
containing 16

L1 STRUCTURE UPLOADED

=> s l1  
SAMPLE SEARCH INITIATED 16:45:06 FILE 'CASREACT'  
SCREENING COMPLETE - 375 REACTIONS TO VERIFY FROM 18 DOCUMENTS

100.0% DONE 375 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 6339 TO 8661  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 ( 0 REACTIONS)

=> s l1 full

FULL SEARCH INITIATED 16:45:12 FILE 'CASREACT'

SCREENING COMPLETE - 7002 REACTIONS TO VERIFY FROM 321 DOCUMENTS

100.0% DONE 7002 VERIFIED

4 HIT RXNS

3 DOCS

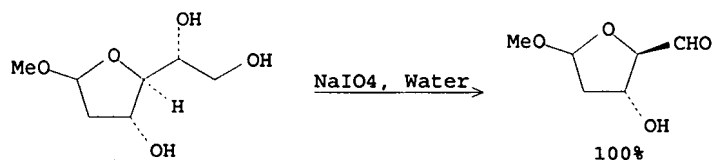
SEARCH TIME: 00.00.05

L3 3 SEA SSS FUL L1 ( 4 REACTIONS)

=> d l3 1-3

L3 ANSWER 1 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 24

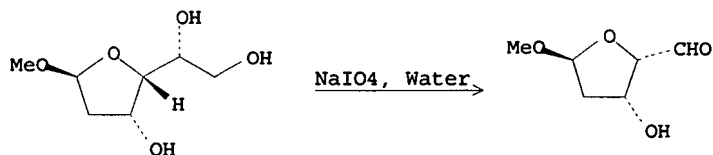


REF: PCT Int. Appl., 2005044832, 19 May 2005

CON: STAGE(1) <0 deg C; 30 minutes, <10 deg C

L3 ANSWER 2 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

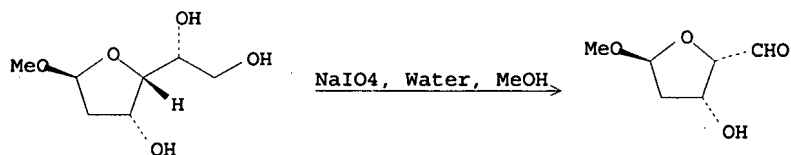
RX(2) OF 15



REF: Carbohydrate Research, 181,, 125-34; 1988

L3 ANSWER 3 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 39



REF: Journal of the American Chemical Society, 107(18), 5283-5; 1985

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

122.13

122.34

FILE 'CAPLUS' ENTERED AT 16:45:29 ON 12 JUN 2007

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=> s 13

L4 3 L3

=> d 14 1-3 ibib hitstr

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:429422 CAPLUS

DOCUMENT NUMBER: 142:463961

TITLE: Process for the preparation of 1-chloro-3,5-di-O-acyl-2-deoxy-L-ribofuranoside derivatives from 2-deoxy-D-galactose via stereoselective chlorination reaction

INVENTOR(S): Tamerlani, Giancarlo; Bartalucci, Debora; Salsini, Liana; Rapaccini, Silvia

PATENT ASSIGNEE(S): Inalco S.p.A., Italy

SOURCE: PCT Int. Appl., 17 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.             | KIND   | DATE   | APPLICATION NO.  | DATE       |
|------------------------|--|--|------------------|------------|
| WO 2005044832          | A1   | 20050519   | WO 2004-EP52900  | 20041110   |
| W:                     | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW |  |                  |            |
| RW:                    | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG   |  |                  |            |
| CA 2545437             | A1   | 20050519   | CA 2004-2545437  | 20041110   |
| EP 1699805             | A1   | 20060913   | EP 2004-818161   | 20041110   |
| R:                     | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS   |  |                  |            |
| CN 1878782             | A  | 20061213   | CN 2004-80033026 | 20041110   |
| JP 2007510696          | T  | 20070426   | JP 2006-538856   | 20041110   |
| US 2007083041          | A1   | 20070412   | US 2006-578800   | 20060509   |
| PRIORITY APPLN. INFO.: |  |  | IT 2003-FI288    | A 20031110 |
|                        |  |  | WO 2004-EP52900  | W 20041110 |
| OTHER SOURCE(S):       | CASREACT 142:463961; MARPAT 142:463961   |  |                  |            |
| REFERENCE COUNT:       | 1  | THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT |                  |            |

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1989:173573 CAPLUS

DOCUMENT NUMBER: 110:173573

TITLE: Synthesis of 2-deoxy-D-arabino-(6-13C)hexose

AUTHOR(S): Walker, Thomas E.; Ehler, Deborah S.; Unkefer, Clifford J.

CORPORATE SOURCE: Los Alamos Natl. Lab., Los Alamos, NM, 87545, USA

SOURCE: Carbohydrate Research (1988), 181, 125-34

CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:173573

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1985:560278 CAPLUS

DOCUMENT NUMBER: 103:160278

TITLE: Total synthesis of the cytochrome P-450 epoxxygenase metabolites 5(R),6(S)-, 5(S),6(R)-, and 14(R),15(S)-epoxyeicosatrienoic acid (EET) and hydration products 5(R),6(R)- and 14(R),15(R)-dihydroxyeicosatrienoic acid (DHET)

AUTHOR(S): Moustakis, Christine A.; Viala, Jacques; Capdevila, Jorge; Falck, J. R.

CORPORATE SOURCE: Health Sci. Cent., Univ. Texas, Dallas, TX, 75235, USA

SOURCE: Journal of the American Chemical Society (1985), 107(18), 5283-5

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 103:160278

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

4.01

126.35

STN INTERNATIONAL LOGOFF AT 16:46:12 ON 12 JUN 2007